

# Two-loop matching conditions for $\overline{\text{MS}}$ parton densities

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We discuss how the the operator product expansion (OPE) can be used to derive asymptotic expressions for certain integrals. This yields operator matrix elements (OME's) which determine the matching conditions for  $\overline{\text{MS}}$  parton densities across heavy flavour thresholds. Then we construct four and five-flavour densities from a three-flavour set via the evolution of the AP equation using LO and NLO splitting functions.

It is well known that  $\alpha_s(\mu^2, n_f, \Lambda(n_f))$  in pQCD requires matching conditions as the scale  $\mu$  crosses flavour matching points. At these points the number of light-flavours  $n_f$  changes by unity so the QCD scale parameter  $\Lambda(n_f)$  in the solution of the differential equation for the  $\beta$  function is redefined to make the running coupling continuous. When heavy quarks are included another scale  $m$ , the mass of the heavy quark, enters and the matching conditions are more complicated. The precise relations which need to be satisfied are given in [ 1], [ 2]. In order lowest order pQCD one can choose to make the  $\alpha_s$  continuous across heavy flavour thresholds at  $\mu = m$ . However this does not hold in higher order pQCD as the matching conditions in the  $\overline{\text{MS}}$  scheme then contain non-logarithmic terms. Hence there is a discontinuity in  $\alpha_s$  at  $\mu = m$ .

Recently the analogous problem of deriving the two-loop matching conditions on parton densities as the mass factorization scale crosses the heavy flavour thresholds has been solved in [ 3]. The way this was done is as follows. We examined the large  $Q^2$  limit of the heavy quark coefficient functions which appear in NLO perturbation expressions for heavy quark extrinsic pair production in deep inelastic scattering. These quantities are functions of the virtuality of the photon probe  $\sqrt{Q^2}$ , the mass of the heavy quark  $m$ , the renormalization scale  $\mu$ , which is chosen equal to the mass factorization scale, and the partonic Bjorken scaling variable  $z$ . The number of heavy

$D^*$  mesons produced in deep inelastic scattering can be derived by convoluting these heavy  $(c - \bar{c})$  quark coefficient functions with appropriate combinations of three-flavour light parton densities (u,d,s and g) and with heavy  $(c - \bar{c})$  quark fragmentation functions [ 4]. Note that the heavy  $c - \bar{c}$  pair only appears in the final state. Unfortunately we do not have analytic expressions for all these heavy quark coefficient functions. Some only exist as two-dimensional integrals over very complicated expressions. However there are convenient tables for all of them in [ 5].

In the limit  $Q^2 \gg m^2$  the complicated integrals in the heavy quark coefficient functions reduce to terms with powers of  $\ln(Q^2/\mu^2)$  and  $\ln(\mu^2/m^2)$  multiplied by functions of the variable  $z$ . These results can be reexpressed as convolutions of light-mass coefficient functions  $\mathcal{C}(z, Q^2/\mu^2)$  which contain the terms with powers in  $\ln(Q^2/\mu^2)$  and OME's  $A(z, \mu^2/m^2)$  which contain the powers in  $\ln(\mu^2/m^2)$ . The way we evaluated these OME's is described in [ 6] so we only give an outline here. We wrote the heavy quark coefficient functions in terms of dispersion integrals for off-shell forward Compton scattering as is normally done for the OPE in deep inelastic scattering. We then changed variables to write the dispersion integral in terms of a variable  $z'$  which is between zero and unity. Next we expanded the denominator in a Taylor series in  $z'$ . To take the limit  $Q^2 \gg m^2$  of the dispersion integral we add and subtract the same dispersion integral where we take the limit  $Q^2 \gg m^2$  in the integrand. This integrand con-

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tains the OPE of the standard heavy quark (Q) nonsinglet and singlet operators in pQCD taken between states with momentum  $k$ , namely

$$\langle Q(k) | O_{Q,\mu_1,\mu_2,\dots,\mu_n}(0) | Q(k) \rangle. \quad (1)$$

The heavy quark operator

$$O_{Q,\mu_1,\mu_2,\dots,\mu_n}(x) = \bar{\psi}(x) \gamma_{\mu_1} D_{\mu_2} \dots D_{\mu_n} \psi(x), \quad (2)$$

is a gauge invariant operator containing the heavy quark field  $\psi(x)$  and the covariant derivative  $D_\mu = \partial_\mu + igA_\mu$ . It can be shown that the original integral minus the integral involving the OPE does not contain any mass singularities as  $m \rightarrow 0$  so it cannot depend on the heavy quark mass  $m$  and therefore only contains terms with powers of  $\ln(Q^2/\mu^2)$ . Hence the integrals which contain the evaluation of the OME's in the OPE yield all the terms containing powers of  $\ln(\mu^2/m^2)$ . This means that analytic expressions for the two-loop OME's with one heavy quark loop and light-quark or gluon incoming and outgoing states contain the information we require to extract the  $A(z, \mu^2/m^2)$ . Of course the actual evaluation of the five OME's which exist in order  $\alpha_s^2$  requires the introduction of infrared and ultraviolet regulators, the use of gauge invariant operators, contractions with light-like four vectors to make the projections and  $\overline{\text{MS}}$  renormalization. The results of this analysis are encapsulated in expressions like

$$\begin{aligned} \tilde{A}_{Qq}^{\text{PS},(2)}(z, \mu^2/m^2) &= A_1(z) \ln^2(\mu^2/m^2) \\ &+ A_2(z) \ln(\mu^2/m^2) + A_3(z), \end{aligned} \quad (3)$$

where

$$\begin{aligned} A_1(z) &= C_F T_f [-8(1+z) \ln z \\ &- 16/(3z) - 4 + 4z + 16z^2/3], \end{aligned} \quad (4)$$

$$\begin{aligned} A_2(z) &= C_F T_f [-8(1+z) \ln^2 z \\ &+ (8 + 40z + 64z^2/3) \ln z \\ &+ 160/(9z) - 16 + 48z - 448z^2/9], \end{aligned} \quad (5)$$

$$\begin{aligned} A_3(z) &= C_F T_f \{ (1+z) [32S_{1,2}(1-z) \\ &+ 16 \ln z \text{Li}_2(1-z) \\ &- 16\zeta(2) \ln z - 4/3 \ln^3 z] \end{aligned}$$

$$\begin{aligned} &+ (32/(3z) + 8 - 8z - 32z^2/3) \text{Li}_2(1-z) \\ &+ (-32/(3z) - 8 + 8z + 32z^2/3) \zeta(2) \\ &+ (2 + 10z + 16z^2/3) \ln^2 z \\ &- (56/3 + 88z/3 + 448z^2/9) \ln z - 448/(27z) \\ &- 4/3 - 124z/3 + 1600z^2/27 \}. \end{aligned} \quad (6)$$

The tilde indicates that an overall factor of  $n_f$  has been extracted from the function and the (2) in the superscript means this is the second order term in an expansion in  $a_s = \alpha_s/(4\pi)$ . The five functions  $\tilde{A}_{Qq}^{\text{PS},(2)}(z, \mu^2/m^2)$ , where PS denotes pure singlet under the flavour group (i.e., no non-singlet projection exists),  $\tilde{A}_{Qg}^{\text{S},(2)}(z, \mu^2/m^2)$ , where S denotes singlet under the flavour group,  $A_{gg,Q}^{\text{S},(2)}(z, \mu^2/m^2)$ ,  $A_{qq,Q}^{\text{S},(2)}(z, \mu^2/m^2)$ , and  $A_{qq,Q}^{\text{NS},(2)}(z, \mu^2/m^2)$  where NS denotes non-singlet under the flavour group, which exist in order  $\alpha_s^2$  pQCD are given in [3]. Alternative discussions of their derivation and use are given in [7]. Note that they contain nonlogarithmic terms such as  $A_3(z)$  in Eq.(6) in order  $\alpha_s^2$  so there is no scale  $\mu$  where we can make them all vanish. Since we know the four-flavour light mass coefficient functions  $\mathcal{C}(z, Q^2/\mu^2)$  in order  $\alpha_s^2$  [8] we can analytically evaluate the convolutions with the appropriate  $A$ 's to obtain asymptotic expressions for the heavy quark coefficient functions. They were given in [9]. As far as this workshop is concerned we would like to point out that this "inverse mass factorization method" is an elegant use of the OPE to obtain asymptotic expansions of integrals.

Normally parton densities are fitted to specific functions of  $x$  at a scale  $\mu$  and the AP equations then govern the evolution of these densities to other scales. Suppose one begins with a three-flavour set containing densities for u,d,s quarks and the gluon g. Then the above results allow one to define four-flavour parton densities at scales  $\mu \geq m_c$  from the input set of three-flavour densities in fixed-order perturbation theory (FOPT). Let the  $\otimes$  symbol denote the convolution integral  $f \otimes g = \int f(x/y)g(y)dy/y$ , where  $x \leq y \leq 1$ , then we define the charm density

$$f_{c+\bar{c}}(n_f + 1, \mu^2) =$$

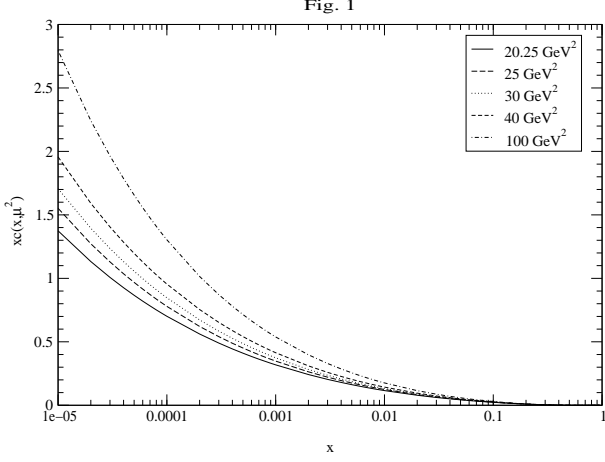


Figure 1.  $xc_{\text{NNLO}}(5, x, \mu^2)$  in the range  $10^{-5} < x < 1$  for  $\mu^2 = 20.25, 25, 30, 40$  and  $100$  in units of  $(\text{GeV}/c^2)^2$ .

$$\begin{aligned}
& a_s(n_f, \mu^2) \tilde{A}_{Qg}^S\left(\frac{\mu^2}{m_c^2}\right) \otimes f_g^S(n_f, \mu^2) \\
& + a_s^2(n_f, \mu^2) \left[ \tilde{A}_{Qq}^{\text{PS}}\left(\frac{\mu^2}{m_c^2}\right) \otimes f_q^S(n_f, \mu^2) \right. \\
& \left. + \tilde{A}_{Qg}^S\left(\frac{\mu^2}{m_c^2}\right) \otimes f_g^S(n_f, \mu^2) \right], \quad (7)
\end{aligned}$$

the singlet gluon density

$$\begin{aligned}
& f_g^S(n_f + 1, \mu^2) = f_g^S(n_f, \mu^2) \\
& + a_s(n_f, \mu^2) A_{gg,Q}^S\left(\frac{\mu^2}{m_c^2}\right) \otimes f_g^S(n_f, \mu^2) \\
& + a_s^2(n_f, \mu^2) \left[ A_{gq,Q}^S\left(\frac{\mu^2}{m_c^2}\right) \otimes f_q^S(n_f, \mu^2) \right. \\
& \left. + A_{gg,Q}^S\left(\frac{\mu^2}{m_c^2}\right) \otimes f_g^S(n_f, \mu^2) \right], \quad (8)
\end{aligned}$$

and the light mass quark densities

$$\begin{aligned}
& f_{k+\bar{k}}(n_f + 1, \mu^2) = f_{k+\bar{k}}(n_f, \mu^2) \\
& + a_s^2(n_f, \mu^2) A_{qq,Q}^{\text{NS}}\left(\frac{\mu^2}{m_c^2}\right) \otimes f_{k+\bar{k}}(n_f, \mu^2), \quad (9)
\end{aligned}$$

for  $n_f = 3$  and  $m_c^2 \leq \mu^2 < m_b^2$ . Note that we have suppressed the  $x$  dependence to make the notation more compact. These expressions were used in [7] to construct a variable flavour number

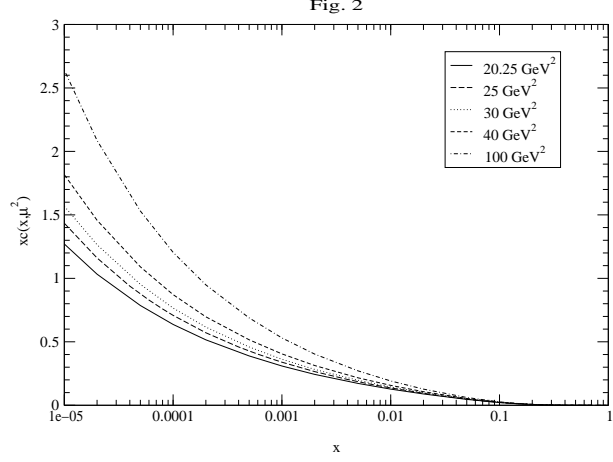


Figure 2. Same as Fig.1 for the NLO results from MRST98 set 1.

scheme (VFNS) for the heavy quark contributions to the deep inelastic structure functions.

Note however that the above procedure does not resum the potentially large terms in  $\ln(\mu^2/m_c^2)$  which are explicitly left in the parton densities. To do this we need to evolve the above densities via the AP equation rather than using FOPT. This is new work in [10] using three-flavour densities at small scales from [11]. The latter LO and NLO densities are started at very small scales  $\mu_0$  below the mass of the charmed quark. Hence three flavor evolution proceeds from the initial  $\mu_0^2$  to the scale  $\mu^2 = m_c^2 = 1.96 (\text{GeV}/c^2)^2$ . In this region  $\alpha_s$  is large so we had to be very careful to get numerically accurate solutions of the evolution equation. Fortunately there are standard inputs and tables in [12] with which we could compare the parton densities from our evolution code. We chose the matching scale  $\mu$  at the mass of the charm quark  $m_c$  so that all the  $\ln(\mu^2/m_c^2)$  terms in the OME's vanish at this point leaving only the nonlogarithmic pieces in the order  $\alpha_s^2$  OME's to contribute to the right-hand-sides of Eqs. (7), (8) and (9). Note that the LO and NLO charm densities vanish at the scale  $\mu = m_c$  since

$$\tilde{A}_{Qg}^{S,(1)}(z, \mu^2/m^2) = 4T_f(z^2 + (1-z)^2) \ln(\mu^2/m^2), \quad (10)$$

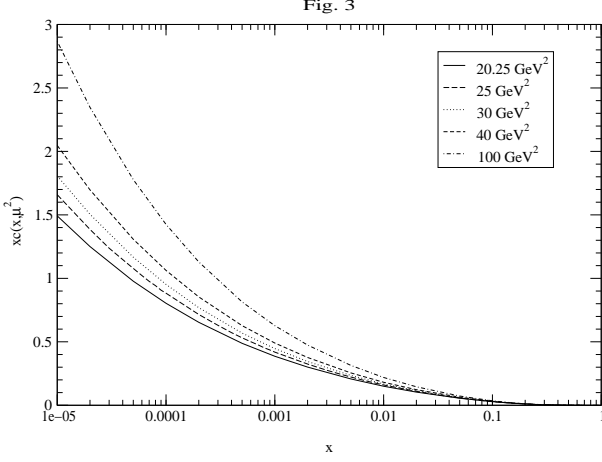


Figure 3. Same as Fig.1 for the NLO results from CTEQ5HQ.

does not have a non-logarithmic term. The NNLO charm density starts off with a finite  $x$ -dependent shape in order  $a_s^2$  determined by

$$f_{c+\bar{c}}(n_f + 1, m_c^2) = a_s^2(n_f, m_c^2) \left[ \tilde{A}_{Qq}^{\text{PS}}(1) \otimes f_q^S(n_f, m_c^2) + \tilde{A}_{Qg}^S(1) \otimes f_g^S(n_f, m_c^2) \right], \quad (11)$$

with  $n_f = 3$ . Hence the OME's provide the boundary condition for the evolution of the (massless) charm density. Also note that we ordered the terms on the right-hand-side of Eq.(11) in powers of  $\alpha_s$  so that the result contains a product of NLO OME's and LO parton densities, although this is not evident here. The result is then strictly order  $a_s^2$  and should be multiplied by order  $a_s^0$  coefficient functions when forming the zero-mass variable flavour number scheme (ZM-VFNS) charm density contribution to the deep inelastic structure functions.

The four-flavour gluon density is also generated at the matching point in the same way. At  $\mu = m_c$  we define

$$f_g^S(n_f + 1, m_c^2) = f_g^S(n_f, m_c^2) + a_s^2(n_f, m_c^2) \left[ A_{gg,Q}^S(1) \otimes f_g^S(n_f, m_c^2) + A_{gg,Q}^S(1) \otimes f_g^S(n_f, m_c^2) \right]. \quad (12)$$

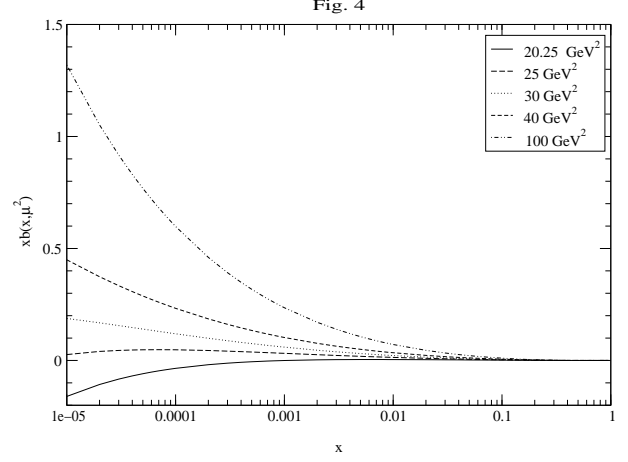


Figure 4.  $xb_{\text{NNLO}}(5, x, \mu^2)$  in the range  $10^{-5} < x < 1$  for  $\mu^2 = 20.25, 25, 30, 40$  and  $100$  in units of  $(\text{GeV}/c^2)^2$ .

The four-flavor light quark (u,d,s) densities are generated using

$$f_{k+\bar{k}}(n_f + 1, m_c^2) = f_{k+\bar{k}}(n_f, m_c^2) + a_s^2(n_f, m_c^2) A_{qq,Q}^{\text{NS}}(1) \otimes f_{k+\bar{k}}(n_f, m_c^2). \quad (13)$$

The *total* four-flavor singlet quark density follows from the sum of Eqs.(11) and (13).

Next the resulting four-flavor densities are evolved from their boundary values using the four-flavor evolution kernels in the AP equations in either LO or NLO up to the scale  $\mu^2 = 20.25 (\text{GeV}/c^2)^2$ . The bottom quark density is then generated at this point using

$$f_{b+\bar{b}}(n_f + 1, m_b^2) = a_s^2(n_f, m_b^2) \left[ \tilde{A}_{Qq}^{\text{PS}}(1) \otimes f_q^S(n_f, m_b^2) + \tilde{A}_{Qg}^{(S)}(1) \otimes f_g^S(n_f, m_b^2) \right], \quad (14)$$

and the five-flavour gluon and light quark densities (which now include charm) are generated using Eqs. (12) and (13) with  $n_f = 4$  and replacing  $m_c^2$  by  $m_b^2$ . Therefore only the nonlogarithmic terms in the order  $a_s^2$  OME's contribute to the matching conditions on the bottom quark density. Then all the densities are evolved up to higher  $\mu^2$  as a five-flavor set with either LO or NLO splitting functions.

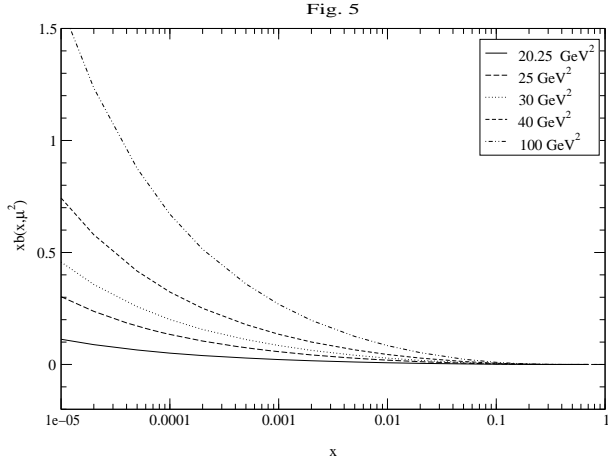


Figure 5. Same as Fig.4 for the NLO results from MRST98 set 1.

The above formulae and their evolution with LO and NLO splitting functions have been implemented in a C++ computer code [10] to yield the CS parton density set. They were used in the construction of two VFNS for the charm quark contribution to the deep inelastic structure functions in [13]. Note that approximate expressions for the three loop splitting functions are now available in [14]. When NNLO parton densities are available from fits to experimental data we can incorporate them into our computer program.

As an illustration we would like to compare the charm and bottom quark densities in the CS [10], MRST98 [15] and CTEQ5 [16] sets. The latter two sets work with order  $\alpha_s$  matching conditions so the parton densities are continuous across heavy flavour thresholds. The MRST98 sets use a procedure proposed in [17], while the CTEQ5 sets use the different ACOT procedure in [18]. Here we show the five-flavor densities. In the CS set they start at  $\mu^2 = m_b^2 = 20.25 \text{ GeV}^2$ . At this scale the charm densities in the CS, MRST98 (set 1) and CTEQ5HQ sets are shown in Figs.1,2,3 respectively. Since the CS charm density starts off negative for small  $x$  at  $\mu^2 = m_c^2 = 1.96 \text{ GeV}^2$  (see the plots in [10]) it is smaller than the corresponding CTEQ5HQ density. At larger  $\mu^2$  all the CS curves in Fig.1 are below those for CTEQ5HQ in Fig.3 although the differences are small. In

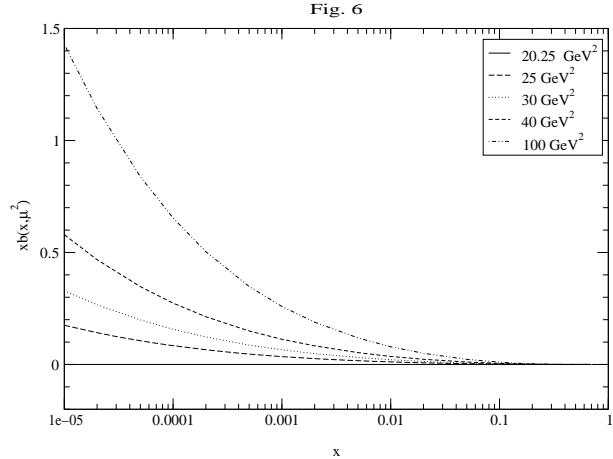


Figure 6. Same as Fig.4 for the NLO results from CTEQ5HQ.

general the CS c-quark densities are more equal to those in the MRST98 (set 1) in Fig.2.

At the matching point  $\mu^2 = 20.25 \text{ GeV}^2$  the b-quark density also starts off negative at small  $x$  as can be seen in Fig.4, which is a consequence of the explicit form of the OME's in [3]. At  $O(\alpha_s^2)$  the nonlogarithmic terms do not vanish at the matching point and yield a finite function in  $x$ , which is the boundary value for the evolution of the b-quark density. This negative start slows down the evolution of the b-quark density at small  $x$  as the scale  $\mu^2$  increases. Hence the CS densities at small  $x$  in Fig.4 are smaller than the MRST98 (set 1) densities in Fig.5 and the CTEQ5HQ densities in Fig.6 at the same values of  $\mu^2$ . The differences between the sets are still small, of the order of five percent at small  $x$  and large  $\mu^2$ . This will lead to differences in cross sections for processes involving incoming b-quarks at the Tevatron.

We suspect that the differences between these results for the c and b-quark densities are primarily due to the different gluon densities in the three sets rather than the effects of the different boundary conditions. This could be checked theoretically if both LO and NLO three-flavor sets were provided by MRST and CTEQ at small scales. We note that CS uses the GRV98 LO and NLO gluon densities, which are rather steep in  $x$  and generally larger than the latter sets

at the same values of  $\mu^2$ . Since the discontinuous boundary conditions suppress the charm and bottom densities at small  $x$ , they enhance the gluon densities in this same region (in order that the momentum sum rules are satisfied). Hence the GRV98 three flavour gluon densities and the CS four and five flavor gluon densities are generally larger than those in MRST98 (set 1) and CTEQ5HQ. Unfortunately experimental data are not yet precise enough to decide which set is the best one.

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